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STRUCTURE FILE UPDATES: 02 DEC 94 HIGHEST RN 159344-42-0

DICTIONARY FILE UPDATES: 08 DEC 94 HIGHEST RN 159344-42-0

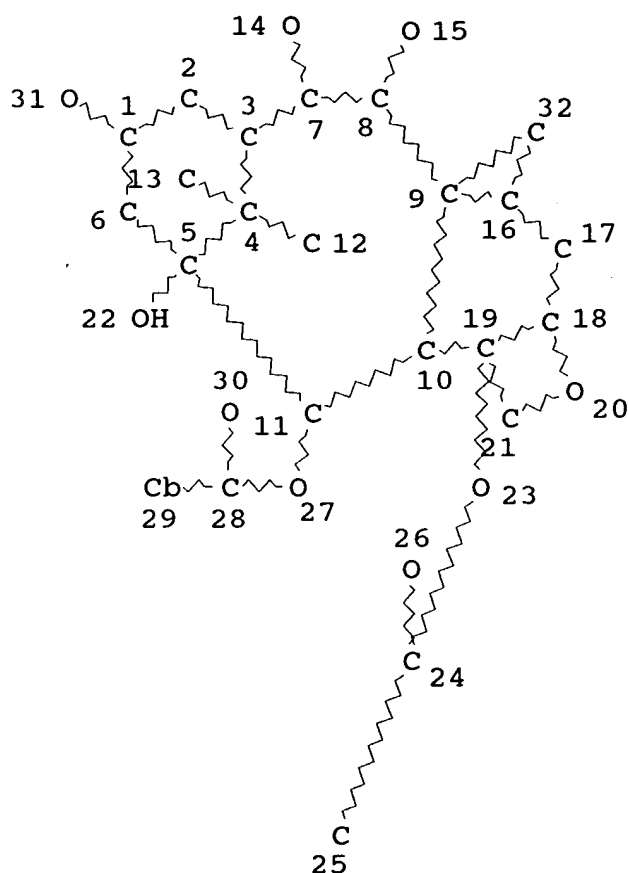
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=> d que 15

L3

STR



NODE ATTRIBUTES:

CONNECT IS E1 RC AT 15

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 7 8 9 10 11

GGCAT IS UNS AT 29

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS UNLIMITED AT 7 8 9 10 11

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

621

L5 87 SEA FILE=REGISTRY SSS FUL L3

87 structures from the query

=> file hca

FILE 'HCA' ENTERED AT 15:55:33 ON 09 DEC 94

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FILE COVERS 1967 - 26 Nov 1994 (941126/ED) VOL 121 ISS 22

=> d his 16

(FILE 'REGISTRY' ENTERED AT 15:49:31 ON 09 DEC 94)
SAVE L5 TRIN162/AL6 FILE 'HCA' ENTERED AT 15:51:47 ON 09 DEC 94
6 S L5*6 CA ref's from the 87 structure*

=> d 16 1-6 all

L6 ANSWER 1 OF 6 HCA COPYRIGHT 1994 ACS

AN 121:109331 HCA

TI Preparation of fluorotaxols as antitumor agents

IN Chen, Shu Hui; Farina, Vittorio; Kant, Joydeep; Vyas, Dolatrai M.

PA Bristol-Myers Squibb Co., USA

SO U.S., 21 pp. Cont.-in-part of U.S. Ser. No. 6,423, abandoned.

CODEN: USXXAM

PI US 5294637 A 940315

AI US 93-62687 930520

PRAI US 92-907261 920701

US 92-996455 921224

US 93-6423 930119

US 93-29819 930311

DT Patent

LA English

IC ICM A01N043-02

ICS C07D305-00

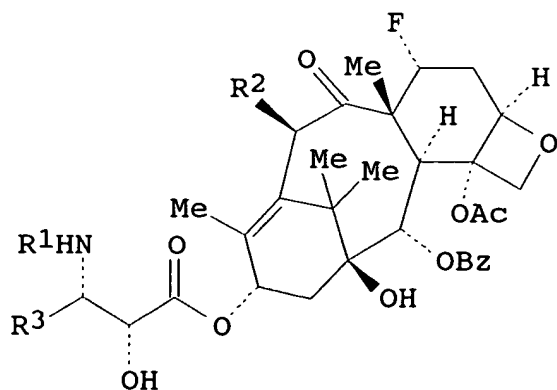
NCL 514449000

CC 30-20 (Terpenes and Terpenoids)

Section cross-reference(s): 1

OS MARPAT 121:109331

GI



I

4022

AB Title compds. [I; R1 = COR,CO2R; R = (cyclo)alkyl, alkenyl, Ph, etc.; R2 = H, OH, OR, O2CR, etc.; R3 = (cyclo)alkyl, alkenyl, WR4, etc.; R4 = Ph, naphthyl, furyl, thienyl, etc.; W = bond, alkenylene, (CH2)1-6] were prepd. Thus, taxol was converted to N-debenzoyl-N-tert-butoxycarbonyl-7.alpha.-fluorotaxol which gave mean survival time 147% of controls in M109 lung carcinoma inoculated-mice receiving 40mg/kg i.p. on days 5 and 8 post-implant.

ST fluorotaxol prepn antitumor agent; taxol fluoro prepn antitumor agent

IT Neoplasm inhibitors
(fluorotaxols)

IT 150799-82-9P 150799-84-1P 156294-33-6P
156294-35-8P 156294-36-9P
(formation of, in prepn. of antitumor agent)

IT 92-29-5P, Hydrobenzamide 132127-34-5P 133066-59-8P
144764-08-9P 144764-09-0P 144790-00-1P 144790-01-2P
147650-53-1P 148121-24-8P 148121-25-9P 148121-26-0P
148205-41-8P 148930-30-7P, 2'-O-Benzylloxycarbonyltaxol
149140-54-5P 149198-47-0P 153652-60-9P 156294-32-5P
156294-34-7P 156294-37-0P 156294-38-1P 156294-39-2P
156294-40-5P 156294-41-6P 156294-42-7P 156294-43-8P
156294-44-9P 156294-46-1P 156294-47-2P 156294-48-3P
156294-49-4P 156294-50-7P 156294-51-8P 156406-30-3P
156406-31-4P 156406-32-5P
(prepn. and reaction of, in prepn. of fluorotaxol antitumor agent)

IT 100-52-7P, Benzaldehyde, reactions
(prepn. of)

IT 153652-63-2P, 7.alpha.-Fluorotaxol 156294-27-8P 156294-28-9P
156294-29-0P 156294-30-3P 156294-31-4P 156294-52-9P
156294-53-0P
(prepn. of, as antitumor agent)

IT 494-47-3, Hydrofuramide 13831-31-7, Acetoxyacetyl chloride
33069-62-4, Taxol 39994-75-7, L-Threonine methyl ester
hydrochloride 78432-77-6, 10-Desacetyltaxol 114261-50-6,
Hydrothienamide 115437-18-8
(reaction of, in prepn. of fluorotaxol antitumor agent)

L6 ANSWER 2 OF 6 HCA COPYRIGHT 1994 ACS

AN 121:109329 HCA

TI reparation of 7,8-cyclopropataxanes as antitumor agents

IN Chen, Shu Hui; Farina, Vittorio

PA Bristol-Myers Squibb Co., USA

SO Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW

PI EP 577083 A1 940105

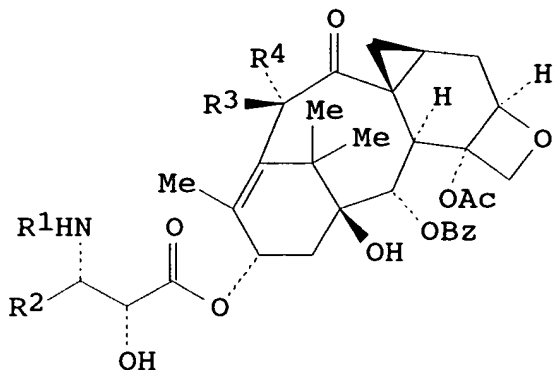
DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE

AI EP 93-110375 930629

PRAI US 92-907261 920701
US 92-995443 921223
US 92-996455 921224
US 93-6423 930119
US 93-29819 930311
US 93-62687 930520

DT Patent

LA English
 IC ICM C07D305-14
 ICS A61K031-335
 CC 30-20 (Terpenes and Terpenoids)
 Section cross-reference(s): 1
 OS MARPAT 121:109329
 GI



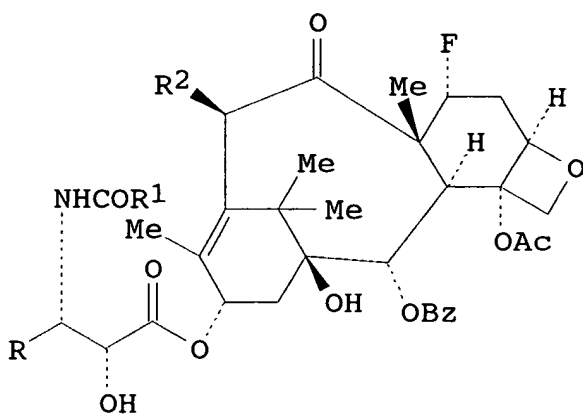
I

AB Tile compds. [I; R1 = alkanoyl, Bz, etc.; R2 = (cyclo)alkyl, alkenyl, aryl, etc.; R3 = H, OH, alkoxy-carbonyloxy, etc.; R4 = H; R3R4 = O] were prepd. Thus, 7-epi-hydroxytaxol was converted in 3 steps to 7-deoxy-8-desmethyl-7,8-cyclopropataxol which had IC50 of 0.183.µg/mL against HCT-116/VM46 human colon carcinoma cells in vitro.

ST cyclopropataxane prepn antitumor
 IT Neoplasm inhibitors
 (cyclopropataxanes)

IT	150799-83-0P	153652-63-2P	156478-93-2P	156478-94-3P
	(formation of, in prepn. of antitumor agent)			
IT	105377-71-7P	115437-18-8P	132127-34-5P	144764-08-9P
	144764-09-0P	144790-01-2P	147650-53-1P	148121-24-8P
	148121-25-9P	148121-26-0P	148121-28-2P	148205-41-8P
	148930-30-7P	148969-14-6P	149140-51-2P	149140-52-3P
	149140-53-4P	149140-54-5P	149198-47-0P	149249-91-2P
	150799-82-9P	153652-60-9P	156294-32-5P	
	156294-33-6P	156294-34-7P	**156294-35-8P***	
	156478-90-9P	156478-91-0P	156478-92-1P	
	156557-30-1P			
	(prepn. and reaction of, in prepn. of antitumor agent)			
IT	150799-84-1P	156294-36-9P	156478-95-4P	
	156478-96-5P			
	(prepn. of, as antitumor agent)			
IT	100-52-7, Benzaldehyde, reactions	32981-86-5, 10-Desacetylbaccatin		
III	33069-62-4, Taxol	39994-75-7, L-Threonine methyl ester		
	hydrochloride	78432-77-6, 10-Deacetyltaxol	78454-17-8	
	105454-04-4, 7-epi-Taxol			
	(reaction of, in prepn. of antitumor agent)			

AN 121:83684 HCA
 TI Preparation of fluorotaxols with antitumor activity
 IN Chen, Shu Hui; Farina, Vittorio; Vyas, Dolatrai; Kant, Joydeep
 PA Bristol-Myers Squibb Co., USA
 SO Eur. Pat. Appl., 45 pp.
 CODEN: EPXXDW
 PI EP 577082 A1 940105
 DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT,
 SE
 AI EP 93-110374 930629
 PRAI US 92-907261 920701
 US 92-995443 921223
 US 92-996455 921224
 US 93-6423 930119
 US 93-29819 930311
 US 93-62687 930520
 DT Patent
 LA English
 IC ICM A61K031-335
 ICS C07D305-14
 CC 30-20 (Terpenes and Terpenoids)
 Section cross-reference(s): 1
 OS MARPAT 121:83684
 GI



I

AB Title compds. [I; R = (cyclo)alkyl, alkenyl, alkynyl, RxW; R1 = (cyclo)alkyl, alkenyl, alkynyl, Ph, etc.; R2 = H, OH, alkoxy(carbonyl), phenoxy(carbonyl), etc.; Rx = Ph, furyl, thienyl, naphthyl, etc.; W = bond, (CH2)1-6, alkeylene] were prepd. Thus, taxol was condensed with ClCO2CH2Ph and the product treated with DAST to give, after deprotection, I (R = R1 = Ph, R2 = OAc). I (R = Ph, R1 = OCMe3, R2 = OAc) gave mean survival of M109 lung carcinoma-implanted mice 147% that of controls at 40mg/kg i.p. on days 5 and 8 post-implant.
 ST fluorotaxol prepn antitumor
 IT Neoplasm inhibitors
 (fluorotaxols)
 IT 92-29-5P, Hydrobenzamide 132127-34-5P 133066-59-8P
 144764-08-9P 144764-09-0P 144790-01-2P 147650-53-1P
 148121-24-8P 148121-25-9P 148121-26-0P 148121-28-2P

425

148205-41-8P 148930-30-7P, 2'-O-(Benzyloxycarbonyl)taxol
149140-54-5P 149198-47-0P **150799-82-9P**
150799-84-1P 153652-60-9P 156294-32-5P
156294-33-6P 156294-34-7P **156294-35-8P**
156294-36-9P 156294-37-0P 156294-38-1P 156294-39-2P
156294-40-5P 156294-41-6P 156294-42-7P 156294-43-8P
56294-44-9P 156294-45-0P 156294-46-1P 156294-47-2P
156294-48-3P 156294-49-4P 156294-50-7P 156294-51-8P
156406-29-0P 156406-30-3P 156406-31-4P 156406-32-5P
(prepn. and reaction of, in prepn. of antitumor agent)
IT 153652-63-2P 156294-27-8P 156294-28-9P 156294-29-0P
156294-30-3P 156294-31-4P 156294-52-9P 156294-53-0P
(prepn. of, as antitumor agent)
IT 98-88-4, Benzoyl chloride 100-52-7, Benzaldehyde, reactions
494-47-3, Hydrofuramide 13831-31-7, Acetoxyacetyl chloride
33069-62-4, Taxol 39994-75-7, L-Threonine methyl ester
hydrochloride 78432-77-6, 10-Desacetyltaxol 114261-50-6
115437-18-8
(reaction of, in prepn. of antitumor agent)
L6 ANSWER 4 OF 6 HCA COPYRIGHT 1994 ACS
AN 120:299016 HCA
TI Synthesis of Ring B-Rearranged Taxane Analogs
AU Klein, Larry L.; Maring, Clarence J.; Li, Leping; Yeung, Clinton M.;
Thomas, Sheela A.; Grampovnik, David J.; Plattner, J. J.; Henry,
Rodger F.
CS Anti-Infective Division, Abbott Laboratories, Abbott Park, IL,
60064, USA
SO J. Org. Chem. (1994), 59(9), 2370-3
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1, 75
OS CASREACT 120:299016; CJACS-IMAGE; CJACS
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Reaction of the C-7 hydroxyl group on the 9-dihydrotaxane skeleton,
e.g. I, with triflic anhydride causes a major skeletal rearrangement
to occur leading to contraction of ring B. A side product, II, is
the formation of a ring C-fused cyclopropane structure. The
requisite C-13 phenylisoserinate side chains are appended via an
initial deacylation of the C-13 acetate followed by reacylation and
deprotection. These rearranged compds., e.g. III (R = Bz, CO₂CMe₃)
and IV show very similar structural features with the parent
9-dihydrotaxane skeleton and also retain biol. activity.
ST taxane diterpene rearranged analog biol activity; dihydrotaxane
skeleton rearrangement triflic anhydride; ring contraction
dihydrotaxane skeleton; cyclopropanation dihydrotaxane skeleton
triflic anhydride; phenylisoserinate deriv acylation baccatin analog
IT Crystal structure
(of baccatin III rearranged analogs)

426

IT Rearrangement
(of dihydrotaxane skeleton with triflic anhydride)

IT Neoplasm inhibitors
(taxol rearranged analogs)

IT Diterpenes and Diterpenoids
(taxane, rearranged analogs, prepn. and antitumor activity of)

IT 133066-61-2 152089-12-8
(acylation by, of baccatin III rearranged analogs)

IT 27548-93-2DP, Baccatin III, analogs
(prepn. and acylation of, with azetidiones taxol analogs from)

IT 154854-31-6P
(prepn. and acylation of, with azetidiones, taxol analogs from)

IT 33069-62-4DP, analogs 148584-53-6DP, 9-Dihydrotaxol, analogs
154854-32-7P **154854-37-2P** 154854-38-3P
(prepn. and antitumor activity of)

IT 154854-36-1P
(prepn. and attempted acylation of, with azetidiones)

IT 154854-33-8P 154854-39-4P
(prepn. and rearrangement of, with triflic anhydride)

IT 154854-30-5P
(prepn. and reductive deacetylation of, in synthesis of taxol analogs)

IT **154854-34-9P**
(prepn. and regioselective deacetylation of, in synthesis of taxol analogs)

IT **154854-35-0P**
(prepn. and silylation of, in synthesis of taxol analogs)

IT 142203-65-4, 13-Acetyl-9-dihydrobaccatin III
(rearrangement of, with triflic anhydride)

L6 ANSWER 5 OF 6 HCA COPYRIGHT 1994 ACS

AN 120:218230 HCA

TI On the reaction of taxol with DAST

AU Chen, Shu Hui; Huang, Stella; Farina, Vittorio

CS Bristol-Myers Squibb Pharm. Res. Inst., Wallingford, CT, 06492-7660, USA

SO Tetrahedron Lett. (1994), 35(1), 41-4
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

OS CASREACT 120:218230

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Treatment of 2'-Cbz-taxol (I) with DAST yields several interesting new products, including 7- α -fluoro deriv. II (R = CO₂CH₂Ph) and a cyclopropane-contg. product, III (R = CO₂CH₂Ph). II (R = H) and III (R = H) showed excellent ability to polymerize tubulins in vitro and displayed potent toxicity vs HCT-116 (no data).

ST txol reaction DAST diethyaminosulfur trifluoride

IT Fluorination

427

Rearrangement
(in reaction of taxol and derivs. with DAST)
IT Tubulins
(taxol deriv. polymn. promoter)
IT Neoplasm inhibitors
(taxol derivs. (no data))
IT 7782-41-4
(fluorination, in reaction of taxol and derivs. with DAST)
IT 150799-82-9P 150799-83-0P 153652-60-9P 153652-61-0P
(prepn. of, by reaction of taxol deriv. with DAST)
IT 153652-62-1P
(prepn. of, by reaction of taxol with DAST)
IT 153652-64-3P 153652-65-4P
(prepn. of, via reaction of taxol deriv. with DAST)
IT 150799-84-1P 153652-63-2P
(prepn., tubulin polymn., and cytotoxicity of)
IT 33069-62-4 148930-30-7
(reactant, reaction of taxol and derivs. with DAST)
IT 38078-09-0, DAST
(reagent, reaction of taxol and derivs. with DAST)

L6 ANSWER 6 OF 6 HCA COPYRIGHT 1994 ACS
AN 119:226216 HCA
TI Serendipitous synthesis of a cyclopropane-containing taxol analog
via anchimeric participation of an unactivated angular methyl group
AU Chen, Shu Hui; Huang, Stella; Wei, Jianmei; Farina, Vittorio
CS Bristol-Myers Squibb Pharm. Res. Inst., Wallingford, CT, 06492-7660,
USA
SO J. Org. Chem. (1993), 58(17), 4520-1
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1
OS CASREACT 119:226216; CJACS-IMAGE; CJACS
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Treatment of a 7-epi-taxol deriv. I with DAST in dichloromethane led
to an unexpected reaction, involving participation of the C(19)-Me
group and clean formation of a cyclopropane ring. A subsequent
reaction leading to A ring contraction to cyclopentene II was also
obsd., but this was controlled by careful monitoring of the reaction
and by introducing a limited amt. of the reagent. The analog of
taxol thus produced, III, was shown to retain a high degree of biol.
activity.
ST epitaxol cyclopropanation ring contraction DAST; taxol analog prepn
biol activity
IT Ring contraction
(cyclopropanation and, during fluorination of epitaxol deriv. by
ethylaminosulfur trifluoride)
IT Neoplasm inhibitors
(deoxytaxol analog)

628

IT Neighboring group participation
(in cyclopropanation of epitaxol deriv. with diethylaminosulfur trifluoride)
IT Fluorination
(of epitaxol deriv. with DAST, cyclopropanation and ring contraction during)
IT Ring closure and formation
(cyclopropanation, ring contraction and, during fluorination of epitaxol deriv. with diethylaminosulfur trifluoride)
IT 148969-14-6
(attempted fluorination of, with diethylaminosulfur trifluoride, cyclopropanation and ring contraction during)
IT 7782-41-4
(fluorination, of epitaxol deriv. with DAST, cyclopropanation and ring contraction during)
IT 33069-62-4DP, deoxyanalogs **150799-84-1P**
(prepn. and antitumor activity of)
IT **150799-82-9P**
(prepn. and hydrogenolysis of)
IT 150799-83-0P
(prepn. of)

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E1 THROUGH E12 ASSIGNED

12 hit RN's from the 6 CA refs

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(FILE 'CAPREVIEWS' ENTERED AT 15:52:39 ON 09 DEC 94)

L7 2 S L5
SET COST OFF

2 Capreview ref's from the structure search

FILE 'REGISTRY' ENTERED AT 15:53:46 ON 09 DEC 94

FILE 'HCA' ENTERED AT 15:55:33 ON 09 DEC 94

SEL HIT RN L6 1-6

679

FILE 'CAPREVIEWS' ENTERED AT 15:57:33 ON 09 DEC 94

=> d 17 1-2 all

L7 ANSWER 1 OF 2 CAPreviews COPYRIGHT 1994 ACS
AN 94:609329 CAPreviews
TI New taxoids, their preparation, and pharmaceutical compositions containing them
IN Bouchard, Herve; Bourzat, Jean-Dominique; Commercon, Alain
PA Rhone Poulenc Rorer SA, Fr.
SO Fr. Demande, 35 pp.
CODEN: FRXXBL
PI FR 2698871 A1 940610
AI FR 92-14813 921209
DT Patent
LA French
IC ICM C07D305-14
ICS A61K031-335
CC 30 (Terpenes and Terpenoids)
Section cross-reference(s): 1
AB Taxoids I [R = H, Ac; R1 = Bz, R2OCO; R2 = alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, bicycloalkyl, Ph, heterocyclyl; Ar = aryl] were prepd. (1 example) for use as antitumor agents and antineoplastics, esp. for ovarian cancer. Thus, protected taxotere deriv. II (BOC = Me3COCO; R7 = R10 = CO2CH2CCl3) was deprotected by powd. Zn in AcOH-EtOAc mixt. to give II (R7 = R10 = H), which was treated with (CF3SO2)2O and pyridine in CH2Cl2 to give II (R7 = SO2CF3, R10 = H). The latter was treated with NaN3 in MeCN-THF mixt. and heated to 80.degree., which induced cyclization of the triflate to the 7.beta.,8.beta.-methylene deriv. Subsequent cleavage of the oxazolidine protective function in formic acid and replacement of the BOC group with di-tert-Bu dicarbonate gave final product I (R = H, R1 = BOC, Ar = Ph). Compds. I are said to be at least as active as taxol and taxotere, and were active at 1-10 mg/kg i.p. against melanoma B16 in mice (no addnl. data).
IT RN LIST MAY NOT BE COMPLETE: 358-23-6; 24424-99-5; 143527-76-8; 158811-30-4; 159262-90-5; 159262-91-6; 159262-92-7; 159262-93-8

L7 ANSWER 2 OF 2 CAPreviews COPYRIGHT 1994 ACS
AN 94:392956 CAPreviews
TI Preparation of 7-halo- and 7.beta.,8.beta.-methanotaxols, their antineoplastic use and pharmaceutical composition containing them
IN Hester, Jackson B., Jr.; Johnson, Roy A.; Kelly, Robert C.; Midy, Eldon G.; Skulnick, Harvey I.
PA Upjohn Co., USA
SO PCT Int. Appl., 127 pp.
CODEN: PIXXD2
PI WO 9413655 A1 940623
DS W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, US, US, US, UZ, VN
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
AI WO 93-US11827 931213
PRAI US 92-990579 921215
US 93-13826 930202

430

US 93-76337 930611
US 93-122974 930917
DT Patent
LA English
IC ICM C07D305-14
ICS C07D413-12; C07D263-04
CC 30 (Terpenes and Terpenoids)
Section cross-reference(s): 1, 34, 63
AB This invention provides 7-deoxy-taxol analogs or formula (I). The compds. of formula (I) (including formulate II and III) are useful for the same cancers for which taxol has been shown active, including human ovarian cancer, breast cancer, and malignant melanoma as well as lung cancer, gastric cancer, colon cancer, head and neck cancer, and leukemia.
IT RN LIST MAY NOT BE COMPLETE: 77-74-7; 103-71-9; 501-53-1; 558-42-9; 590-42-1; 1609-86-5; 2094-72-6; 2890-61-1; 3282-30-2; 7693-46-1; 17341-93-4; 17380-62-0; 22509-74-6; 27548-93-2; 32981-85-4; 32981-86-5; 33069-62-4; 78432-77-6; 91352-76-0; 95603-44-4; 99458-15-8; 100431-55-8; 103150-33-0; 114915-13-8; 114915-14-9; 114977-28-5; 115437-21-3; 124605-42-1; 125354-16-7; 133524-70-6; **150799-84-1**; 153652-63-2; 155399-27-2; 155399-30-7; **156294-33-6**; **156294-36-9**; 157240-36-3; 157580-27-3; 157580-31-9; 158809-53-1; **158809-54-2**; 158809-55-3; **158809-56-4**; 158809-57-5; **158809-58-6**; 158809-59-7; 158809-61-1; 158809-62-2; 158809-63-3; 158809-64-4; 158809-65-5; 158809-66-6; 158809-67-7; 158809-68-8; 158809-69-9; 158809-70-2; 158809-71-3; 158809-72-4; 158809-73-5; 158809-74-6; 158809-75-7; 158809-76-8; 158809-77-9; 158809-78-0; 158809-79-1; 158809-80-4; 158809-81-5; 158809-82-6; 158809-83-7; **158809-84-8**; **158809-85-9**; **158809-86-0**; **158809-87-1**; **158809-89-3**; **158809-90-6**; **158809-91-7**; **158809-92-8**; **158809-93-9**; **158809-94-0**; **158809-95-1**; **158809-96-2**; **158809-97-3**; **158809-98-4**; **158809-99-5**; **158810-00-5**; **158810-01-6**; **158810-02-7**; **158810-03-8**; **158810-04-9**; **158810-05-0**; **158810-06-1**; **158810-07-2**; **158810-08-3**; **158810-09-4**; **158810-10-7**; **158810-11-8**; 158810-12-9; 158810-13-0; 158810-14-1; 158810-15-2; 158810-16-3; 158810-17-4; 158810-18-5; 158810-19-6; **158810-20-9**; **158810-21-0**; **158810-22-1**; **158810-23-2**; **158810-24-3**; **158810-25-4**; **158810-26-5**; **158810-27-6**; **158810-28-7**; **158810-29-8**; **158810-30-1**; **158810-31-2**; 158810-32-3; 158810-33-4; 158810-34-5; 158810-35-6; 158810-36-7; 158810-37-8; 158810-38-9; 158810-39-0; 158810-40-3; 158810-41-4; 158810-42-5; 158810-43-6; 158810-44-7; 158810-45-8; 158810-46-9; 158810-47-0; 158810-48-1; 158810-49-2; 158810-50-5; 158810-51-6; 158810-52-7; 158810-53-8; 158810-54-9; 158810-55-0; 158810-56-1; 158810-57-2; 158810-58-3; 158810-59-4; 158810-60-7; 158810-61-8; 158810-62-9; 158810-63-0; 158810-64-1; 158810-65-2; 158810-66-3; 158810-67-4; 158810-68-5; 158810-69-6; 158810-70-9; 158810-71-0; 158810-72-1; 158810-73-2; 158810-74-3; 158810-75-4; 158810-76-5; 158810-77-6; 158810-78-7; 158810-79-8; 158810-80-1; 158810-81-2; 158810-82-3; 158810-83-4; 158810-84-5; 158810-85-6; 158810-86-7; **158810-87-8**; **158810-88-9**; **158810-89-0**;

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158851-95-7

=> sel hit rn 1-2 17
E13 THROUGH E92 ASSIGNED

*hit RN's from these 2 Capreview
Ref 2*

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DICTIONARY FILE UPDATES: 08 DEC 94 HIGHEST RN 159344-42-0

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conducting SmartSELECT searches.

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1 150799-84-1/BI
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632

1 154854-34-9/BI
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 1 156478-96-5/BI
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 /BI OR 156478-95-4/BI OR 156478-96-5/BI)

=> d l8 1-12 ide can

*structures from the
6 CA refs*

L8 ANSWER 1 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN **156478-96-5** REGISTRY
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-,
 12a-(acetyloxy)-1-(benzoyloxy)-1,3,4,7,8,9,9a,10,10a,12,12a,12b-
 dodecahydro-2-hydroxy-5,13,13-trimethyl-7,8-dioxo-2,6-methano-2H-
 cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxet-4-yl ester,
 [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R*),8aS*,9a.alpha.,1
 0a.alpha.,12a.alpha.,12b.alpha.]]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

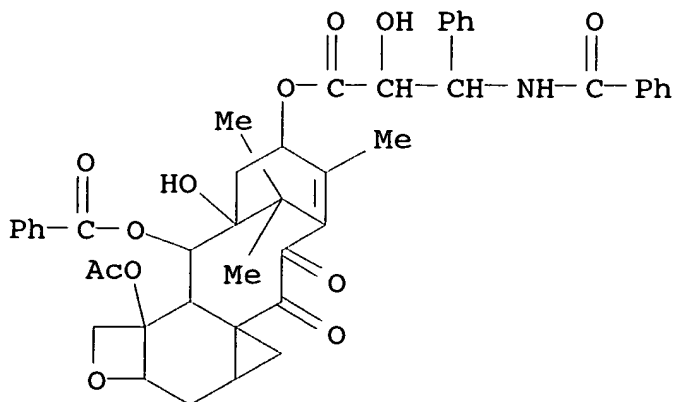
CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
 benzenepropanoic acid deriv. (9CI)

MF C45 H45 N O12

SR CA

LC STN Files: CA

DES *

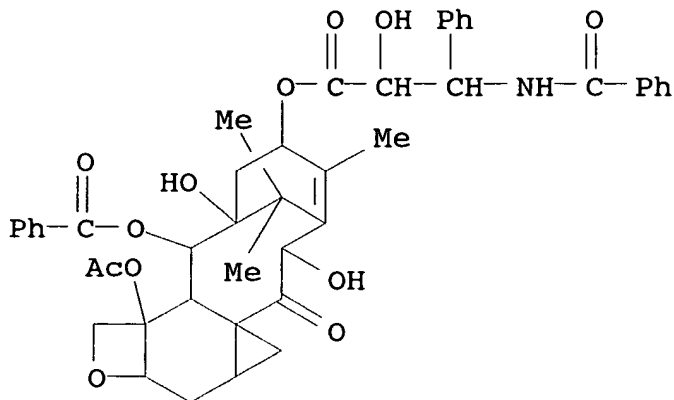


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109329

633

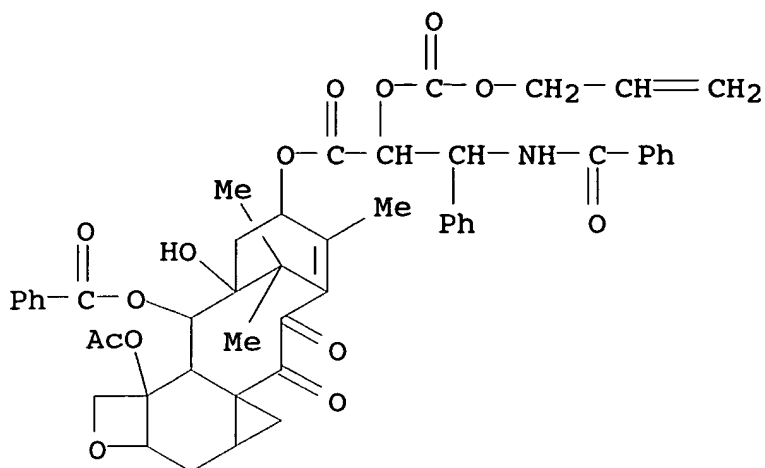
L8 ANSWER 2 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN 156478-95-4 REGISTRY
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-,
 12a-(acetyloxy)-1-(benzoyloxy)-1,3,4,7,8,9,9a,10,10a,12,12a,12b-
 dodecahydro-2,7-dihydroxy-5,13,13-trimethyl-8-oxo-2,6-methano-2H-
 cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxet-4-yl ester,
 [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R*),7.beta.,8aS*,9a.
 alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
 benzenepropanoic acid deriv. (9CI)
 MF C45 H47 N O12
 SR CA
 LC STN Files: CA
 DES *



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109329

L8 ANSWER 3 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN 156478-92-1 REGISTRY
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-[[(2-
 propenyloxy)carbonyl]oxy]-, 12a-(acetyloxy)-1-(benzoyloxy)-
 1,3,4,7,8,9,9a,10,10a,12,12a,12b-dodecahydro-2-hydroxy-5,13,13-
 trimethyl-7,8-dioxo-2,6-methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz
 [1,2-b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.b
 eta.R*),8aS*,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI)
 (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
 benzenepropanoic acid deriv. (9CI)
 MF C49 H49 N O14
 SR CA
 LC STN Files: CA
 DES *



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109329

L8 ANSWER 4 OF 12 REGISTRY COPYRIGHT 1994 ACS

RN **156478-90-9** REGISTRY

CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-[[(2,2,2-trichloroethoxy)carbonyl]oxy]-, 12a-(acetyloxy)-1-(benzoyloxy)-1,3,4,7,8,9,9a,10,10a,12,12a,12b-dodecahydro-2-hydroxy-5,13,13-trimethyl-8-oxo-7-[[(2,2,2-trichloroethoxy)carbonyl]oxy]-2,6-methano-2H-cyclodeca[3,4]cyclopropana[4,5]benz[1,2-b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R*),7.beta.,8aS*,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

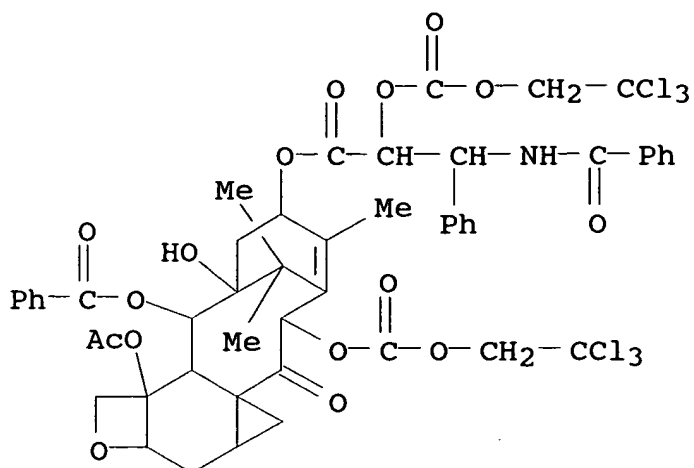
CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropana[4,5]benz[1,2-b]oxete, benzenepropanoic acid deriv. (9CI)

MF C51 H49 Cl6 N O16

SR CA

LC STN Files: CA

DES *



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109329

L8 ANSWER 5 OF 12 REGISTRY COPYRIGHT 1994 ACS

RN 156294-36-9 REGISTRY

CN Benzenepropanoic acid, .beta.-[[(1,1-dimethylethoxy) carbonyl] amino]-
.alpha.-hydroxy-, 7,12a-bis(acetyloxy)-1-(benzoyloxy)-
1,3,4,7,8,9,9a,10,10a,12,12a,12b-doccahydro-2-hydroxy-5,13,13-
trimethyl-8-oxo-2,6-methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-
b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R
),7.beta.,8aS,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

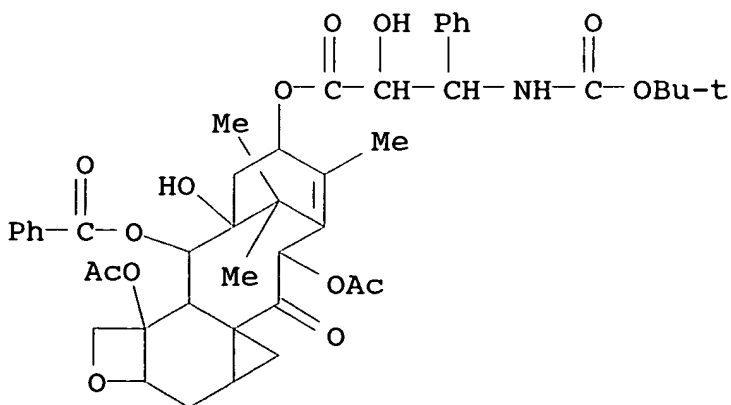
CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
benzenepropanoic acid deriv. (9CI)

MF C45 H53 N O14

SR	CA
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LC STN Files: CA, CAPREVIEWS

DES *



1 REFERENCES IN FILE CAPREVIEWS

3 REFERENCES IN FILE CA (1967 TO DATE)

43 b

REFERENCE 1: P 121:109331

REFERENCE 2: P 121:109329

REFERENCE 3: P 121:83684

L8 ANSWER 6 OF 12 REGISTRY COPYRIGHT 1994 ACS

RN 156294-35-8 REGISTRY

CN Benzenepropanoic acid, .beta.-[[(1,1-dimethylethoxy)carbonyl]amino]-
.alpha.-[(triethylsilyl)oxy]-, 7,12a-bis(acetyloxy)-1-(benzoyloxy)-
1,3,4,7,8,9,9a,10,10a,12,12a,12b-dodecahydro-2-hydroxy-5,13,13-
trimethyl-8-oxo-2,6-methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-
b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R
),7.beta.,8aS,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

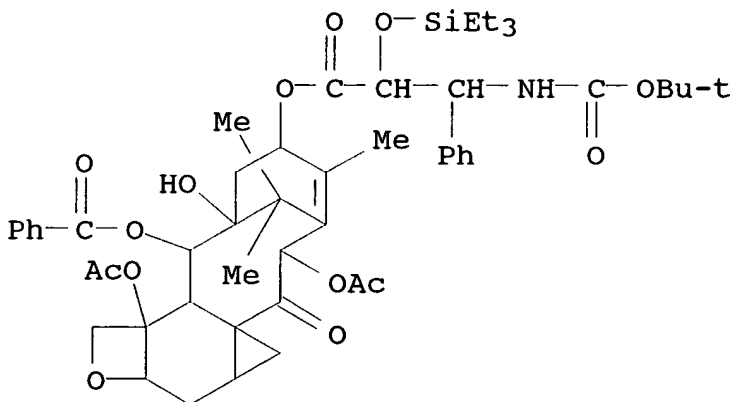
CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
benzenepropanoic acid deriv. (9CI)

MF C51 H67 N O14 Si

SR CA

LC STN Files: CA

DES *



3 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109331

REFERENCE 2: P 121:109329

REFERENCE 3: P 121:83684

L8 ANSWER 7 OF 12 REGISTRY COPYRIGHT 1994 ACS

RN 156294-33-6 REGISTRY

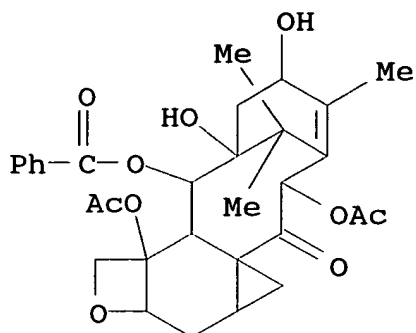
CN 2,6-Methano-8H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxet-8-one,
7,12a-bis(acetyloxy)-1-(benzoyloxy)-1,2,3,4,7,9,9a,10,10a,12,12a,12b-
dodecahydro-2,4-dihydroxy-5,13,13-trimethyl-, [1S-
(1.alpha.,2.alpha.,4.alpha.,7.beta.,8aS*,9a.alpha.,10a.alpha.,12a.al
pha.,12b.alpha.))]- (9CI) (CA INDEX NAME)

MF C31 H36 O10

SR CA

637

LC STN Files: CA, CAPREVIEWS
DES *



1 REFERENCES IN FILE CAPREVIEWS
3 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109331

REFERENCE 2: P 121:109329

REFERENCE 3: P 121:83684

L8 ANSWER 8 OF 12 REGISTRY COPYRIGHT 1994 ACS

RN **154854-37-2** REGISTRY

CN Benzenepropanoic acid, .beta.-[[(1,1-dimethylethoxy)carbonyl]amino]-
.alpha.-hydroxy-, 7,12a-bis(acetyloxy)-1-(benzoyloxy)-
1,3,4,7,8,9,9a,10,10a,12,12a,12b-dodecahydro-2,8-dihydroxy-5,13,13-
trimethyl-2,6-methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-
b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R
),7.beta.,8.alpha.,8aS,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]
]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
benzenepropanoic acid deriv. (9CI)

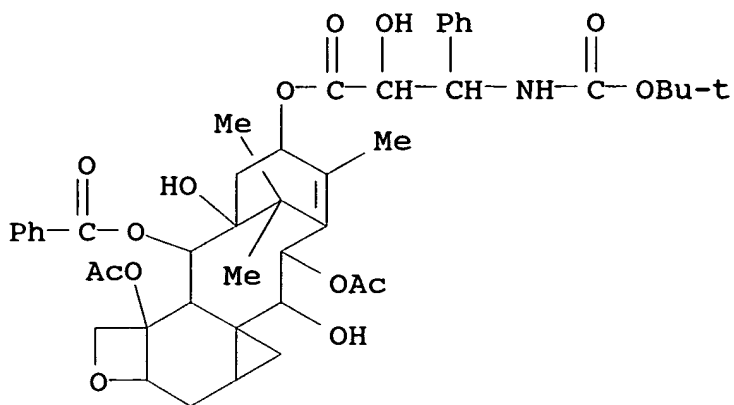
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SR CA

LC STN Files: CA, CASREACT

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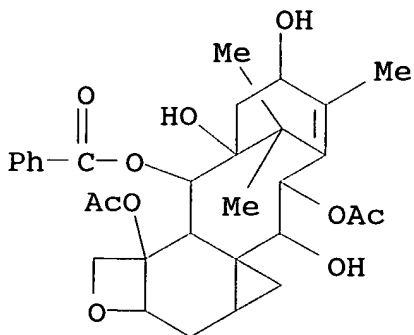
638



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:299016

L8 ANSWER 9 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN **154854-35-0** REGISTRY
 CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete-1,2,4,7,8,12a(12H)-hexol, 1,3,4,7,8,9,9a,10,10a,12b-decahydro-5,13,13-trimethyl-, 7,12a-diacetate 1-benzoate, [1S-(1.alpha.,2.alpha.,4.alpha.,7.beta.,8.alpha.,8aS*,9a.alpha.,10a.alpha.a.,12a.alpha.,12b.alpha.)]- (9CI) (CA INDEX NAME)
 MF C31 H38 O10
 SR CA
 LC STN Files: CA, CASREACT
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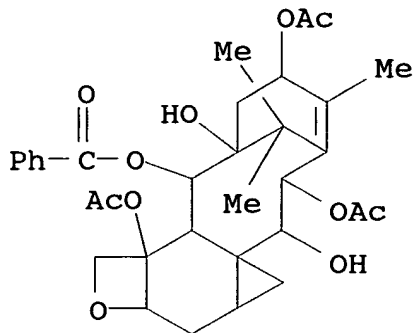
1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:299016

L8 ANSWER 10 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN **154854-34-9** REGISTRY
 CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete-1,2,4,7,8,12a(12H)-hexol, 1,3,4,7,8,9,9a,10,10a,12b-decahydro-5,13,13-trimethyl-, 4,7,12a-triacetate 1-benzoate, [1S-(1.alpha.,2.alpha.,4.alpha.,7.beta.,8.alpha.,8aS*,9a.alpha.,10a.alpha.a.,12a.alpha.,12b.alpha.)]- (9CI) (CA INDEX NAME)

639

MF C33 H40 O11
 SR CA
 LC STN Files: CA, CASREACT
 DES *



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:299016

L8 ANSWER 11 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN **150799-84-1** REGISTRY
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, 7,12a-bis(acetyloxy)-1-(benzoyloxy)-1,3,4,7,8,9,9a,10,10a,12,12a,12b-dodecahydro-2-hydroxy-5,13,13-trimethyl-8-oxo-2,6-methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R*),7.beta.,8aS*,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete, benzenepropanoic acid deriv. (9CI)

MF C47 H49 N O13
 SR CA
 LC STN Files: CA, CAPREVIEWS, CASREACT
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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

1 REFERENCES IN FILE CAPREVIEWS

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REFERENCE 2: P 121:109329

REFERENCE 3: 120:218230

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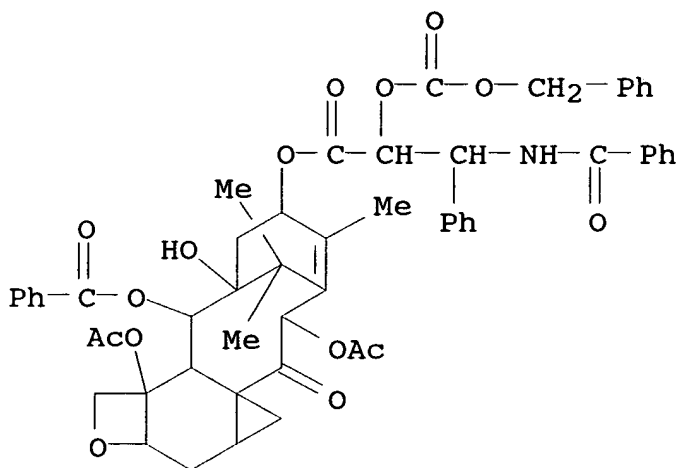
L8 ANSWER 12 OF 12 REGISTRY COPYRIGHT 1994 ACS
 RN **150799-82-9** REGISTRY
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-[[(phenylmethoxy)carbonyl]oxy]-, 7,12a-bis(acetyloxy)-1-(benzoyloxy)-1,3,4,7,8,9,9a,10,10a,12,12a,12b-dodecahydro-2-hydroxy-5,13,13-trimethyl-8-oxo-2,6-methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-

640

b]oxet-4-yl ester, [1S-[1.alpha.,2.alpha.,4.alpha.(.alpha.S*,.beta.R*),7.beta.,8aS*,9a.alpha.,10a.alpha.,12a.alpha.,12b.alpha.]]- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2,6-Methano-2H-cyclodeca[3,4]cyclopropa[4,5]benz[1,2-b]oxete,
benzenepropanoic acid deriv. (9CI)
MF C55 H55 N O15
SR CA
LC STN Files: CA, CASREACT, CHEMINFORMRX
DES *



4 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:109331

REFERENCE 2: P 121:109329

REFERENCE 3: 120:218230

REFERENCE 4: 119:226216

=> d his l8-

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FILE 'REGISTRY' ENTERED AT 15:53:46 ON 09 DEC 94

FILE 'HCA' ENTERED AT 15:55:33 ON 09 DEC 94
SEL HIT RN L6 1-6

FILE 'CAPREVIEWS' ENTERED AT 15:57:33 ON 09 DEC 94
SEL HIT RN 1-2 L7

FILE 'REGISTRY' ENTERED AT 15:58:57 ON 09 DEC 94

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L9 80 S E13-E92

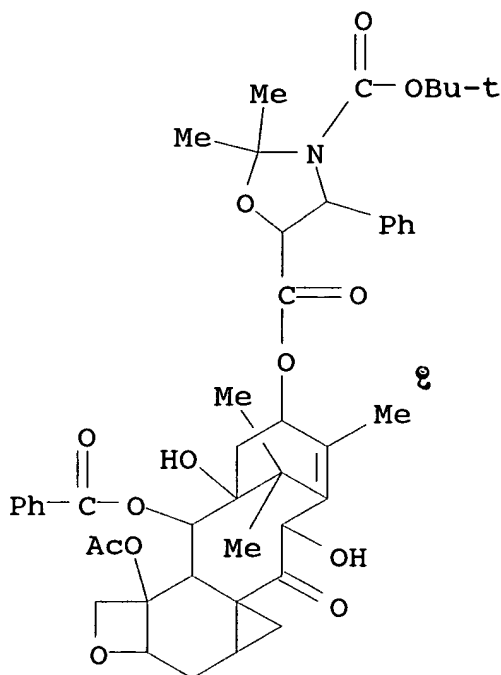
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L10 77 S L9 NOT L8

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L10 ANSWER 1 OF 77 REGISTRY COPYRIGHT 1994 ACS
RN 159262-91-6 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
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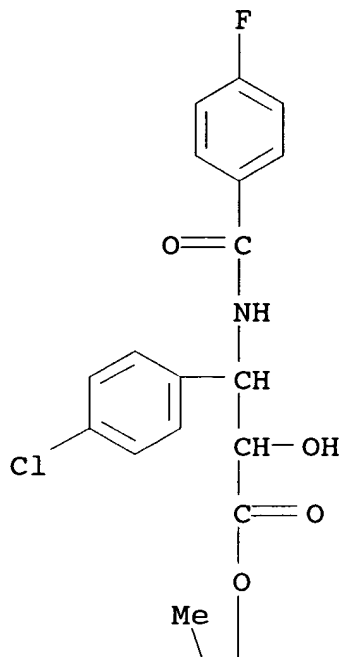


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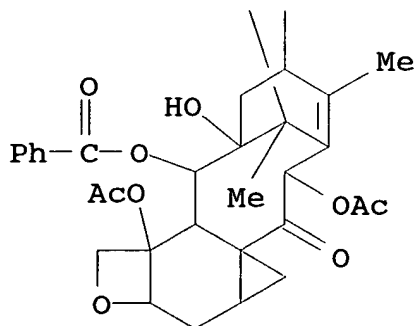
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DES *

1642

PAGE 1-A



PAGE 2-A

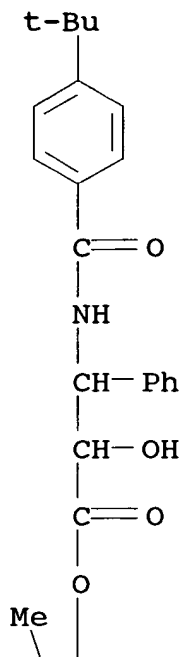


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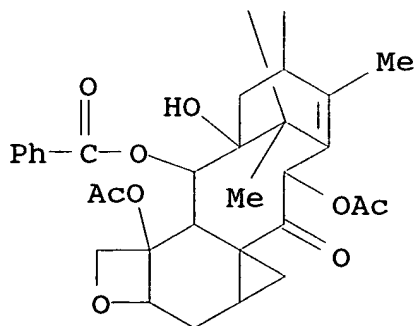
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643

PAGE 1-A



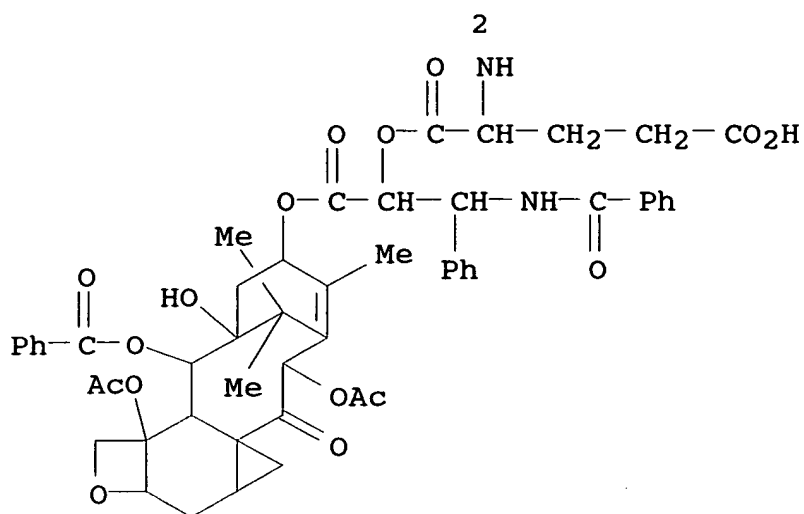
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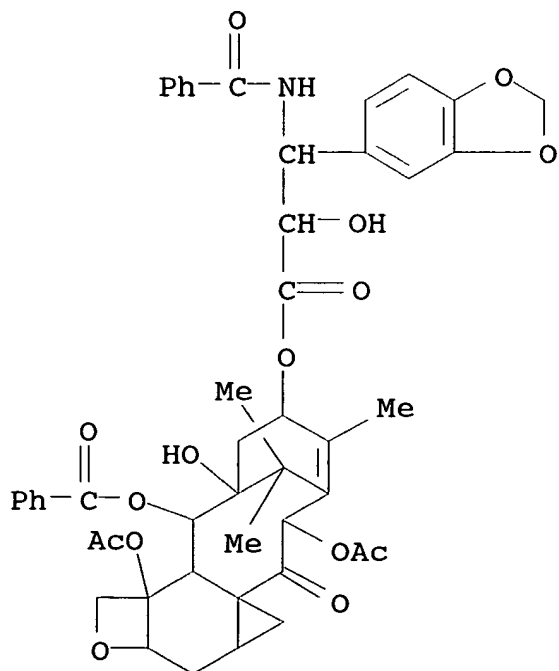
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1 REFERENCES IN FILE CAPREVIEWS

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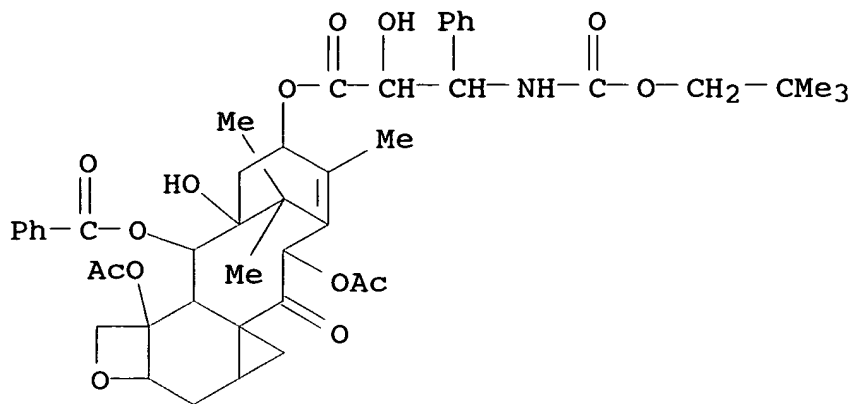


1 REFERENCES IN FILE CAPREVIEWS

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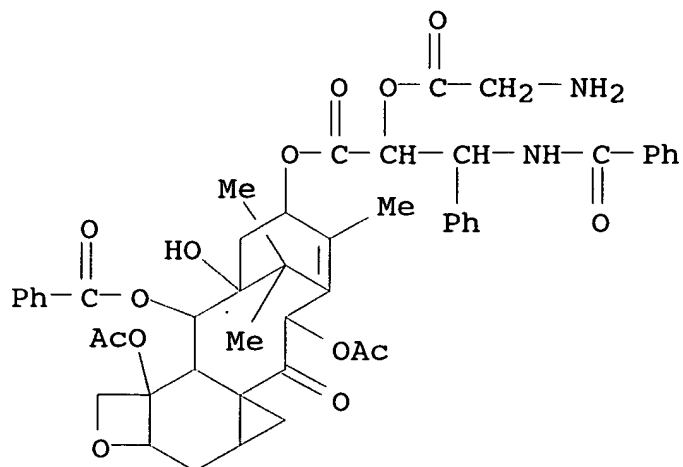
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1 REFERENCES IN FILE CAPREVIEWS

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1 REFERENCES IN FILE CAPREVIEWS

L10 ANSWER 70 OF 77 REGISTRY COPYRIGHT 1994 ACS
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646

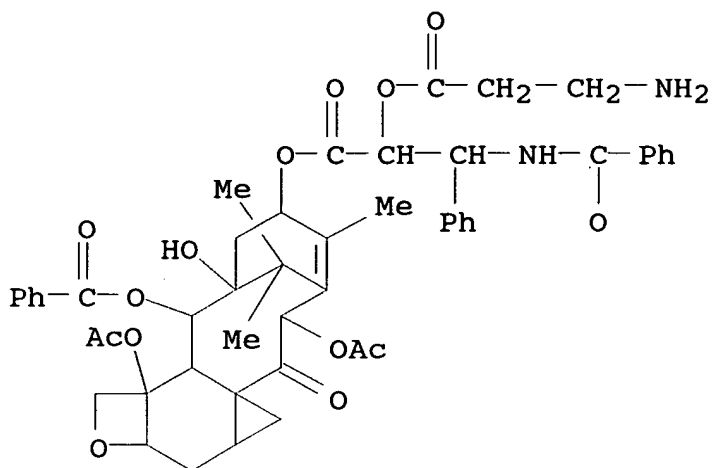
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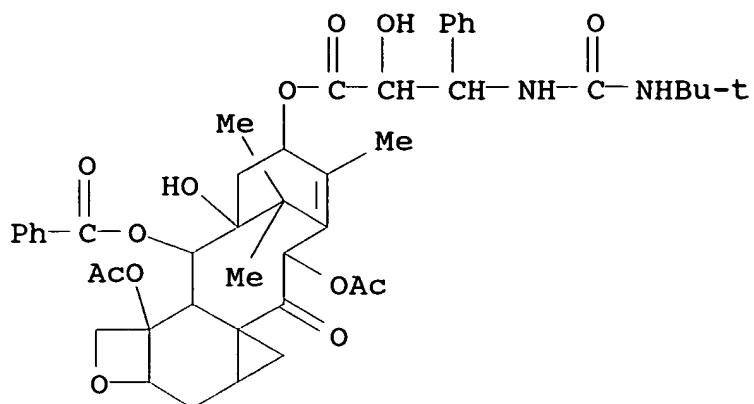
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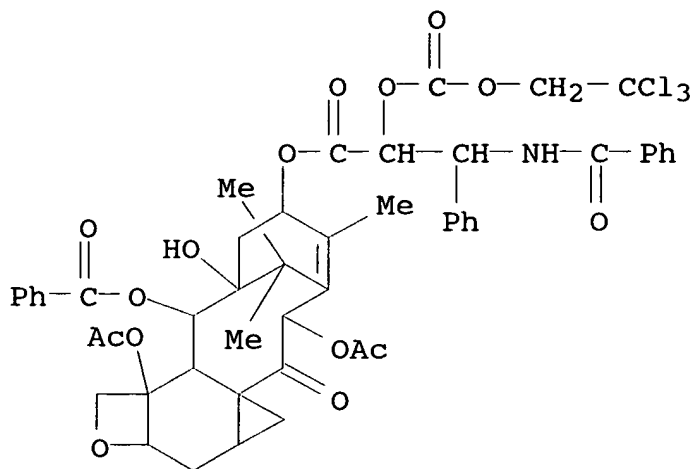
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247



1 REFERENCES IN FILE CAPREVIEWS

L10 ANSWER 77 OF 77 REGISTRY COPYRIGHT 1994 ACS
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1 REFERENCES IN FILE CAPREVIEWS

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